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THEORETICAL STUDIES OF ELECTRON CONDUCTION THROUGH ATTACHING GA--ETC(U)
JUN 82 J N BARDSLEY N00014-82-C-0021
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Preliminary Report

ONR Contract N0014-82-0021

with The University of Pittsburgh

"Theoretical Studies of Electron Conduction Through Attaching Gases"

Period covered: October 1, 1981 - June 30, 1982

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1. Principal Investigator: J. N. Bardsley, Professor of Physics

2. Contract Description: To perform theoretical studies of the motion of electrons through gas mixtures, containing some molecules which easily attach electrons and others that are efficient energy absorbers, in order to provide information about the conduction of electrons in gas discharges. Particular attention will be given to those discharges which are suitable for optically controlled switches or other similar devices being developed in the DOD pulsed power program.

3. Scientific Problem: a) The major goal is to identify a gas mixture with two phases, one of low electrical resistivity and the other of high resistivity, which can be changed rapidly from one phase to the other. The transition could be achieved electrically through changes in the applied voltage, or optically through irradiation by laser light. Such a gas might form the active medium in a diffuse discharge switch that could operate without the movement of electrodes or the addition of large amounts of gas during the opening of the switch.

4. Scientific and Technical Approach:

a) A Monte Carlo simulation code is being developed to permit modelling of arbitrary mixtures in both time-independent and time-dependent situations. The model can incorporate the spatial characteristics of specific devices, but will be first used in simple analyses of homogeneous discharges.

b) Numerical solutions of the Boltzmann equation will be obtained to provide more economical results for equilibrium problems.

c) The atomic collision data required as input to this code must be collected and evaluated. Theoretical estimates must be made for the many processes for which no reliable experimental evidence is available.

d) The influence of high gas densities upon atomic reactions will be studied. This is necessary because many two-body reactions are enhanced by the ambient gas molecules, whereas three-body processes can saturate as the density is increased. These effects are particularly important for recombination and attachment reactions.

e) The characteristics necessary for rapid opening of a switch will be identified and several candidate systems will be selected. The merits of these systems in the conduction phase will then be tested.

This work will be performed in conjunction with the studies being carried out in the Electrical Engineering Department at Texas Technical University. The main contacts with that group are Professors Kunhardt, Schaeffer and Schoenbach.

5. Progress:

a) The Monte Carlo program has been developed to include elastic and inelastic collisions with several molecules, attachment and ionization. It has been tested on N_2, by comparison with the Boltzmann equation solutions of Pitchford and Phelps, and is currently being applied to mixtures of N_2 and HCℓ to test the experimental determinations of attachment rates in such mixtures.

b) A new method for calculating diffusion coefficients has been devised that requires significantly less computer time than previous Monte Carlo methods. At relatively low field strengths our diffusion coefficients appear to be more accurate than our drift velocities.

c) Calculations on high-pressure recombination of electrons with CO_2^+ ions have been completed. The results are in good agreement with experiment, both in regard to the magnitude of the 3-body rate coefficient and the onset of saturation. The maximum rate is $\sim 10^{-4}$ cm^3 s^{-1} which is $\sim$ 250 times higher than the two-body rate measured in low-pressure afterglow experiments.

d) Cross sections for attachment of electrons to HCℓ in specific rotational and vibrational states have been obtained from the measurements of the temperature dependence of the effective attachment cross sections by Allan and Wong. The results confirm the possibility of using HCℓ for optical control of conductivity.

6. Publications:

a) Monte Carlo Calculations of Diffusion Coefficients, B. M. Penetrante and J. N. Bardsley, Lett. Nuovo Cim. 34, 57 (1982).

b) Dissociative Attachment in HCℓ, DCℓ and F_2, J. N. Bardsley and J. M. Wadehra, to be submitted to J. Chem. Phys.

7. Extenuating Circumstances:

The initial budget provided for the partial support of a Research Associate in each year of the contract. Due to delays in this appointment, this category will not be fully spent in the first year, but the funding of a greater percentage of the Research Associate's time will be possible in the 2nd and 3rd years of the contract period.

8. Unspent Funds:

Approximately $16,000 will be unspent as of September 30, 1982, mainly for the reason given above. The availability of these funds guarantees full support of the research associate during the second and third years of this contract. We have also delayed the ordering of some ancillary computing equipment, because of the anticipated offering of a cheaper and more suitable machine.

9. No students have graduate during the contract period.

10. Other Federal support of the principal investigator: Current support

National Science Foundation: Theoretical Physics Program
Grant: PHY8105074
Title: Theoretical Studies of Low Energy Collisions in Atomic Physics
Period: 4/1/81 to 4/30/83
Total Budget: $57,188
Principal Investigator's Effort: 9.8%

Lawrence Livermore National Laboratory (on behalf of DARPA)
Sub-Contract: 5886701
Title: Atomic Processes in Electron Beam Channels
Period: 11/1/81 to 10/31/82
Total Budget: $50,000
Principal Investigator's Effort: 12.5%

No other applications for support are pending.